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AN ALGORITHM FOR DETERMINING DISPERSION AND DOPPLER LINE WIDTHS FROM LIMITED EXPERIMENTAL DATA

R. R. Nigmatullin, N. K. Shcherbakova, and M. Kh. Salakhov†
Department of Physics, Kazan State University, Kazan, 420008 U.S.S.R.

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Abstract—We present an algorithm that allows the efficient determination of the dispersion and Doppler contributions to a Voigt profile from limited experimental data. For this purpose, we use the measured intensity profiles, as well as their first and second derivatives.

ANALYSIS

There has recently been considerable interest in accurate derivations of the dispersion and Doppler components of the Voigt profile from limited data.[1-13] In this paper, we present an algorithm that is useful for this task and which is based on the measured initial profile and on its first and second derivatives. Derivatives of spectra are widely used in derivative spectroscopy.[14]

The Voigt curve may be represented in the form

$$\mathbf{F}(\omega) = \int_0^\infty F(t)\cos(\omega t)\,\mathrm{d}t. \tag{1}$$

where $F(t) = \exp(-at - bt^2/2)$ is the autocorrelation function (ACF), and a and b are the parameters for dispersion and Doppler broadening, respectively. Using the equation for the ACF, we find

$$F'(t) = -(a + bt)F(t). \tag{2}$$

We next write the differential equations for the cosine and sine transforms of $F'(t)$, viz.

$$\int_0^\infty F'(t)\sin(\omega t)\,\mathrm{d}t = -\omega\Phi_c(\omega)$$

$$\int_0^\infty F'(t)\cos(\omega t)\,\mathrm{d}t = -1 + \omega\Phi_s(\omega). \tag{3}$$

Similarly, the transforms for $F(t)$ multiplied by t are

$$\int_0^\infty tF(t)\cos(\omega t)\,\mathrm{d}t = \Phi_s'(\omega),$$

$$\int_0^\infty tF(t)\sin(\omega t)\,\mathrm{d}t = -\Phi_c'(\omega). \tag{4}$$

The following system of equations is obtained for the transforms of the ACF:

$$\left(b\frac{\mathrm{d}}{\mathrm{d}\,\omega} + \omega\right)\Phi_s(\omega) = 1 - a\Phi_c(\omega),$$

$$\left(b\frac{\mathrm{d}}{\mathrm{d}\,\omega} + \omega\right)\Phi_c(\omega) = a\Phi_s(\omega). \tag{5}$$

†To whom all correspondence should be addressed.